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http://www.pdb.org/
info@rcsb.org

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The Protein Data Bank CD-ROM Set

October 2002

The Protein Data Bank (PDB) is the international repository for macromolecular structure data, generated experimentally by X-ray crystallographic and NMR methods, or from theoretical modeling and other techniques. This CD-ROM set contains the macromolecular structure data released through October 1, 2002.

Table of Contents

I. Changes in the CD-ROM Set

18,796 structures are included on this five CD-ROM set.

Changes implemented with this release

1. Theoretical models are now included in a separate /models/ directory on disk 1.

2. With this release, experimental data (structure factor and constraint files) are available separately.

Requests for these data may be submitted at http://www.nist.gov/srd/o_nist801.htm. Users may also request these data by filling out the form in the *Readme.doc* file on disk 1, directory *pub*. and returning it by mail or email.

All CD-ROM services will continue to be available free of charge

For a list of previous changes please consult the *Readme.doc* file on disk 1, directory *pub*.

Your comments and suggestions are welcome. Please send them to ***info@rcsb.org*** or fax to +1 301 975 8717 or mail to PDB, Mail Stop 8314, Gaithersburg, MD, 20899-8314.

II. What is on the CD-ROM set

The Protein Data Bank, the atomic coordinates of the structures of proteins and Nucleic acids, as of October 1, 2002 is contained on this CD-ROM set. The total number of structures in this set is 18,796.

A. Coordinate Data

The purpose of this CD-ROM set is to make available, for research and instruction, the coordinates of experimentally determined macromolecular structures.

If they were deposited, the experimental data - the X-ray structure factor or NMR constraint files used in the structure determination - are available as separate products (see section l).

1. Directory Structure

The coordinate files are found on each disk in a directory named *entries (*except for the theoretical structures found in the *models* directory).

All files are managed in a series of subdirectories that are named so that the directory name is the middle two characters of the PDB ID codes in that directory. For example coordinates file *1dom* would be found in directory *do*. The files are divided across the CD-ROM sets as follows:

Structures

Disk 1 *entries* - two letter directories 00-cm
models - two letter directories 62-zn
Disk 2 *entries* - two letter directories cn-gb
Disk 3 *entries* - two letter directories gc-k7
Disk 4 *entries* - two letter directories k8-tj
Disk 5 *entries* - two letter directories tk-zz

2. Compression

The files have been compressed using the gzip software. Copies of that software (for some UNIX, PC and Mac systems) that can be used to uncompress the files are on DISK 1 in directory */pub/xtrnl_sw*.

A few files in the archive have headers but no coordinates. Those files are not compressed and have an extension of *.noc*.

3. ISO 9660 Constraints

The CD-ROMs are written in standard ISO 9660 format. ISO 9660 format limits file names to eight characters and only allows for one file extension. Consequently after the files were compressed their names were changed to omit the characteristic *.ent* or *.mr* extension and leave only the *.gz* extension so that they could be written to the CD-ROM.

After the files have been transferred to your disk drive and uncompressed, it is possible to add the extension back. The following code for UNIX systems was suggested on earlier copies of the PDB CD-ROM. This example is for the coordinates in directory *entries* that need to have the *.ent* extension.

```
foreach dir (/entries/*)
        foreach lfn ($dir/*)
                mv $lfn $lfn.ent
        end
end
```

B. Other Resources on the CD-ROM sets

In addition to the data directory(s), Disk 1 contains a directory named *pub*. That directory contains an assortment of files and directories as follows:

1. Indices derived from the PDB files

The CD-ROM set contains files relating specific fields in the files to the PDB ID code. The layout of these files varies; some are delimited some are not. To use them refer to the specific file. They are found on disk1 in /pub/resource/index. These files can also be found on the PDB ftp site at ftp.rcsb.org/pub/pdb/derived_data/index

author.idx – idcode, author name

cmpd_res.idx – idcode, resolution, compound name as found in the compound record. The resolution value for entries derived from NMR or theoretical model studies is -1.00. This file is ordered by compound name.

compound.idx – idcode and compound name as found in the compound record.

crystal.idx – idcode, unit cell parameters, space group, Z value.

entries.idx – idcode, header information, accession date, compound, source, author list, resolution, experiment type (sometimes omitted for X-ray).

obsolete.dat – date, obsolete PDB ID, successor PDB ID where appropriate. This file is the same as the file by this name in */pub*.

resolu.idx – idcode, resolution. The resolution value for entries derived from NMR or theoretical model studies is -1.00.

source.idx – idcode, source name as found in the compound records. This file is ordered by source.

2. Deposition Forms

Deposition forms for both X-ray and NMR depositions are found in */pub/dep_nmr.txt* and */pub/dep_xray.txt*. They can also be found online at *ftp.rcsb.org/pub/pdb/doc*. These mmCIF forms can be used to submit NMR or X-ray structures to the PDB as an alternative to the Web-based deposition tool, ADIT (**http://deposit.pdb.org/**).

3. Other information documents

These documents are listed by content - file name in italics - and records or subject matter. On-line availability for each file is given.

a) Holdings – */pub/holdings.doc* or */pub/holdings.htm* – A breakdown of the numbers of PDB structures by experimental technique and molecule type. More extensive PDB growth and holdings information, including graphical depictions, are available on-line at: ***http://www.pdb.org/pdb/holdings.html.***

b) Entry types – */pub/entrytyp.txt* – idcode, type as protein or nucleic acid and experimental technique as *diffraction* for X-ray diffraction, *NMR*, or *model*. That file can be found on-line at: ***ftp://ftp.rcsb.org/pub/pdb/derived_data/.***

c) PDB Contents Guide – */pub/cntnt_21.txt* – Atomic Coordinate Entry Format Description, Version 2.1. A guide to the 1996 version of the PDB file format gives a complete description of the contents of PDB coordinate entry files. Plain text as well as html copies can be found online at:
http://www.rcsb.org/pdb/docs/format/pdbguide2.2/guide2.2_frame.html,

ftp://ftp.rcsb.org/pub/pdb/doc/format_descriptions/Contents_Guide_21.txt,

ftp://ftp.rcsb.org/pub/pdb/doc/format_descriptions/Contents_Guide_21.html.

d) Het dictionary – */pub/hetgroup/het_dict.txt* – picture, residue, het synonym, het name, and formula. This file can also be found at: ***ftp://ftp.rcsb.org/pub/pdb/data/monomers/het_dictionary.txt.***

e) PDB Newsletter – *nwslettr.doc* – The newsletter is available on the CD-ROM set on disk 1, in the directory *pub*, as a text file. All the PDB Newsletters are available on-line at
http://www.pdb.org/pdb/newsletter.html, or
ftp://ftp.rcsb.org/pub/pdb/doc/newsletters.

f) Newsletter subscription information – */pub/nwsl_sub.doc* – email address to sign up for the PDB Newsletter. To subscribe online please go to ***http://www.rcsb.org/pdb/forum.html***.

g) Obsolete records – */pub/obsolete.dat* – date, idcode, and replacement idcode. This list of obsolete data files including structure factors and NMR constraints can be retrieved online from: ***ftp://ftp.rcsb.org/pub/pdb/data/structures/obsolete/***.

h) Sequence – */pub/seqres.txt* – idcode_chainID, molecule type, length of residue sequence, source, sequence. This file can be viewed/retrieved from: ***ftp://ftp.rcsb.org/pub/pdb/derived_data/***.

i) Readme.doc – */pub/readme.doc* – Lists changes recently made or proposed to be made to the PDB CD-ROM set.

j) Changes.doc – */pub/changes.doc* – Lists changes recently made or proposed to be made to the PDB CD-ROM set. Readme.doc and changes.doc are the same file.

k) Document.pdf – */pub/document.pdf* – The PDB CD-ROM documentation is included as an Adobe Acrobat file on disk 1.

4. Software

NOTICE:

The Protein Data Bank does not support any software found on the CD-ROM set. This software has historically been included on the CD-ROM set and is included here for continuity.

Software included on this CD-ROM may require modifications and should be used with caution.

C. Citing the PDB

The contents of PDB are in the public domain, but it is expected that the authors of an entry as well as the PDB be properly cited whenever their work is referred to.

Structures used from the PDB should be cited with the **PDB ID** and the **JRNL** reference.
For example, structure 102L should be referenced as:

PDB ID: 102L
D.W.Heinz,W.A.Baase,F.W.Dahlquist,B.W.Matthews
How Amino-Acid Insertions are Allowed in an Alpha-Helix of T4 Lysozyme.
Nature **361** pp. 561 (1993)

The journal reference for the PDB is:
H.M.Berman, J.Westbrook, Z.Feng, G.Gilliland, T.N.Bhat, H.Weissig, I.N.Shindyalov, P.E.Bourne
The Protein Data Bank
Nucleic Acids Research, **28** pp. 235-242 (2000)

The PDB should also be referenced with the WWW address:
http://www.pdb.org/.

The Brookhaven National Laboratory PDB ceased operation on June 30, 1999.
The original journal reference for the BNL PDB is:
F.C.Bernstein, T.F.Koetzle, G.J.B.Williams, E.F.Meyer Jr, M.D.Brice, J.R.Rodgers, O.Kennard, T.Shimanouchi, M.Tasumi
The Protein Data Bank: a computer-based archival file for macromolecular structures.
J. Mol. Biol. **112** pp. 535-542 (1977)

III. About the PDB

The Protein Data Bank (PDB) is an information portal for researchers and students interested in structural biology. At its center is the PDB archive — the sole international repository for 3-dimensional structure data of biological macromolecules.

The PDB integrates a variety of production-level data and software resources, and shares research results and software. The PDB is dedicated to fostering new scientific advances by providing accurate, consistent, well-annotated 3-D structure data that is delivered in a timely and efficient way to a wide audience.

The contents of the PDB archive contain the structural coordinates and related information about proteins, nucleic acids, and protein-nucleic acid complexes. These structures hold significant promise for the pharmaceutical and biotechnology industries in the search for new drugs and the efforts to understand the mystery of human disease. The understanding of what a structure looks like aids in understanding how it functions.

The PDB is managed by Rutgers, The State University of New Jersey; the San Diego Supercomputer Center at the University of California, San Diego; and the National Institute of Standards and Technology — three members of the Research Collaboratory for Structural Bioinformatics.


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